A glance at the imaginary world of ultracold atoms

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From ultracold atoms to quantum chromodynamics, reliable *ab initio* studies of strongly interacting fermions require numerical methods, typically in some form of quantum Monte Carlo. Unfortunately, (non-)relativistic systems at finite density (spin polarization) generally have a sign problem, such that those *ab initio* calculations are impractical. It is well known, however, that in the relativistic case imaginary chemical potentials solve this problem, assuming the data can be analytically continued to the real axis. Is this feasible for non-relativistic systems? Are the interesting features of the phase diagram accessible in this manner? Introducing complex chemical potentials, for real total particle number and imaginary polarization, the sign problem is avoided in the non-relativistic case. To give a first answer to the above questions, we perform a mean-field study of the finite-temperature phase diagram of spin-1/2 fermions with imaginary polarization.

Ultracold Fermi gases provide an accessible and clean environment to study quantum many-body phenomena [1, 3], ranging from Bose-Einstein condensation (BEC) to Bardeen-Cooper-Schrieffer (BCS) superfluidity. In the dilute limit, where the range of the interaction is smaller than any other scale, a single parameter $(k_{\rm F}a_{\rm s})^{-1}$, where $a_{\rm s}$ is the s-wave scattering length and $k_{\rm F}$ the Fermi momentum, describes the microscopic interactions completely. These are tuned by an external magnetic field in the presence of a Feshbach resonance.

At large $a_{\rm s}$ (in the crossover between BEC and BCS), these systems display universal properties. Here, the scale for all physical observables is set by solely by $k_{\rm F}$ (or, equivalently, the density), which is the only scale left in the problem. Thus, no obvious small expansion parameter exists in this limit, which represents a major challenge for theoretical many-body approaches [2]. Recently, experiments in this so-called unitary regime have achieved high precision [4], potentially allowing to benchmark and improve the available theoretical methods.

Despite tremendous experimental and theoretical advances, our understanding of ultracold Fermi gases at unitarity remains incomplete, most notably for the case of spin-imbalanced systems. For large-enough imbalance, one expects systems to undergo a phase transition from a BCS-type superfluid to a polarized normal gas. Such a transition has been observed in experiments at MIT and Rice university [7] and is in accordance with various theoretical studies [8, 9].

Apart from ultracold gases, a better understanding of spin-imbalanced systems is also of great importance for other research fields. For example, almost all stable nuclei have more neutrons than protons and therefore fall into this class of systems. As a consequence, lattice MC calculations of nuclei [10] therefore suffer from similar problems as *ab initio* lattice calculations of spin-imbalanced Fermi gases.

We shall focus on the $a_{\rm s} \to \infty$ limit for a spin-imbalanced two-component Fermi gas at zero and finite temperature. Unlike previous studies [8, 9], however, we consider a complex-valued chemical potential μ. In *ab initio* MC calculations, this allows to circumvent the sign problem which spoils studies with spin imbalance. This approach parallels that of purely imaginary μ in relativistic quantum field theories, where it enables the analysis of the phase structure of QCD [11] at finite density on the lattice. In that case, the existence of a critical end-point of the line of chiral transitions in the T-μ plane is still an open question, and the answer appears to be out of reach for imaginary-μ approaches [12]. For non-relativistic fermions in the BEC-BCS crossover, on the other hand, the tri-critical end-point of the line of (second-order) superfluid transitions is known to exist. Moreover, our present study suggests that this point might be accessible to lattice calculations by the use of complex-valued chemical potentials.

In this first analysis we employ a mean-field approach, as discussed elsewhere for the case of real-valued μ (see e.g. [9]), to study the phase diagram in the complex-valued case. Although this can only be viewed as a lowest-order approximation, it relies only on a single input parameter (e.g. $k_{\rm F}$) as is the case for the full evaluation of the associated path-integral using, e.g., MC calculations. Thus, our statements do not suffer from a parameter ambiguity but only from an uncertainty associated with the underlying approximation. This can be understood on very general grounds from an analysis of the fixed-point structure of fermionic theories [13].

We begin by discussing a few general aspects of non-relativistic theories with complex-valued chemical poten-

tials. In general, the grand canonical partition function $\mathcal{Z}$ of non-relativistic fermions reads

$$\mathcal{Z}(T,\bar{\mu},h) = \mathrm{Tr}\left[\mathrm{e}^{-\beta(\hat{H}-\bar{\mu}(\hat{N}_\uparrow+\hat{N}_\downarrow)-h(\hat{N}_\uparrow-\hat{N}_\downarrow))}\right], \quad (1)$$

where T is the temperature and $\beta = 1/T$. We shall assume that the Hamiltonian $\hat{H}$ describes the dynamics of a theory with two fermion species, denoted by $\uparrow$ and $\downarrow$, interacting via a two-body interaction. The operators $\hat{N}_{\uparrow,\downarrow}$ denote the particle number associated with each species, and $\mu_{\uparrow,\downarrow}$ are the corresponding chemical potentials. For convenience we have immediately introduced the average chemical potential $\bar{\mu} = (\mu_\uparrow + \mu_\downarrow)/2$ and the asymmetry parameter $h = (\mu_\uparrow - \mu_\downarrow)/2$.

As is well known, MC calculations for unitary fermions can be performed without a sign problem for $h = 0$ (see e.g. Refs. [5, 6]). This is not true in general, however, as polarization yields a sign problem regardless of the form of the interaction. To proceed, we consider an imaginary-valued asymmetry parameter h, which corresponds to studying a theory with complex-valued $\mu_{\uparrow,\downarrow}$, and therefore define $h = \mathrm{i}h_\mathrm{I}$, where h_I is a real quantity. It is easy to verify that MC calculations with imaginary-valued asymmetry can be studied with standard methods without a sign problem: the fermion determinants appearing in the probability measure are complex conjugates of one another. By analytically continuing $\mathcal{Z}(T,\bar{\mu},h_\mathrm{I})$, one obtains $\mathcal{Z}(T,\bar{\mu},h)$, which is the central quantity in studies of imbalanced Fermi gases.

To understand whether the tri-critical end-point is accessible with such an approach, we study the mean-field phase diagram with complex-valued chemical potentials. We compute the mean-field potential for the U(1) order-parameter, from the path-integral representation of $\mathcal{Z}$:

$$\mathcal{Z} = \int \mathcal{D}\psi^\dagger \mathcal{D}\psi\, \mathrm{e}^{-S[\psi^\dagger,\psi]},$$

where

$$S[\psi^\dagger,\psi] = \int d\tau \int d^3x \left\{ \psi^\dagger \left(\partial_\tau - \vec{\nabla}^{\,2} - \bar{\mu}\right)\psi - h\left(\psi_\uparrow^*\psi_\uparrow - \psi_\downarrow^*\psi_\downarrow\right) + \bar{g}(\psi^\dagger\psi)(\psi^\dagger\psi)\right\}, \quad (2)$$

and $\psi^\mathrm{T} = (\psi_\uparrow, \psi_\downarrow)$ and $\bar{g}$ denotes the bare four-fermion coupling. The dimensionless renormalized four-fermion coupling $g \sim \bar{g}\Lambda$ is related to the scattering length a_s by

$$4\pi\Lambda g^{-1} = \left(a_\mathrm{s}^{-1} - c_\mathrm{reg.}\Lambda\right). \quad (3)$$

Here Λ denotes the ultraviolet (UV) cutoff and the constant $c_\mathrm{reg.} > 0$ depends on the regularization scheme. We use units such that $2m = 1$, where m is the fermion mass. We represent the interaction via an auxiliary scalar field $\varphi \sim g_\varphi\, \psi_\uparrow\psi_\downarrow$, where the parameter g_φ is chosen to reproduce the four-fermion term in the action. Fermions can then be integrated out straightforwardly,

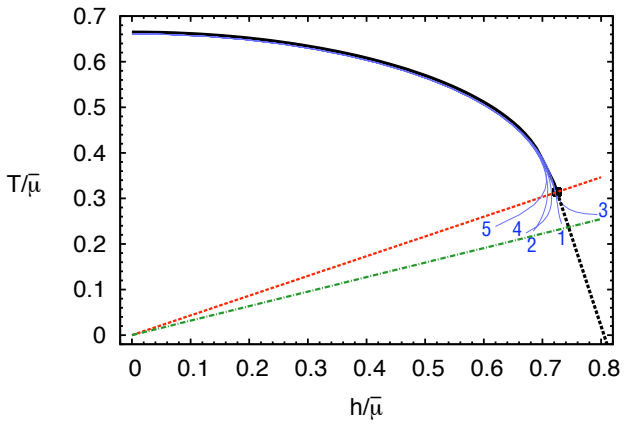

Figure 1. (color online) Phase diagram of an ultracold Fermi gas at unitarity in the (T,h) plane. The solid (black) curve is a line of second-order phase transitions, which ends at a tri-critical point $(h_\mathrm{cp}/\bar{\mu}, T_\mathrm{cp}/\bar{\mu})$ and is followed by a line of first-order transitions (see e.g. Refs. [9]). The (red) dashed line is $T/\bar{\mu} = (T_\mathrm{cp}/h_\mathrm{cp})h/\bar{\mu}$ and the (green) dashed-dotted line is $\pi T/\bar{\mu} = h/\bar{\mu}$. The (light-blue) thin curves are possible analytic continuations obtained from Padé approximants of order $N_\mathrm{max} = 1, 2, \ldots, 5$ (indicated by the numbers), see text.

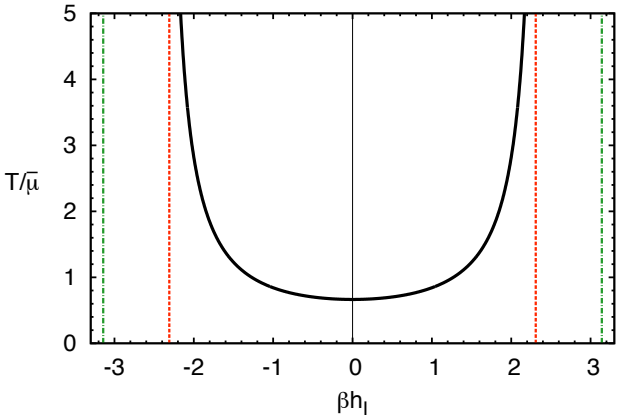

Figure 2. (color online) Phase diagram in the (T,h_I) plane. The solid line is a line of second-order phase transitions below which the fermion gap is finite. The (red) dashed and (green) dash-dotted lines are as in Fig. 1, with h_I replacing h. Between the (red) dashed lines and the (green) dash-dotted lines there is a region with $T_\mathrm{c} \to \infty$ for $\bar{\mu} > 0$. For $\bar{\mu} < 0$, however, T_c remains finite.

as the resulting action is quadratic in those fields, which yields the order-parameter potential:

$$\beta U(\varphi) = -2\beta\bar{\mu}|\varphi|^2 - \int \frac{d^3q}{(2\pi)^3} \ln\left[\frac{1}{2}\left(\cosh(\beta h) + \cosh\left(\beta\sqrt{(\vec{q}^{\,2}-\bar{\mu})^2 + g_\varphi^2|\varphi|^2}\right)\right)\right]. \quad (4)$$

This potential is directly related to the grand canonical potential: $\Omega = VU(\varphi_0)$, where V is the volume of the system and φ_0 denotes the mean-field value of φ that minimizes the potential. In that state, $g_\varphi^2|\varphi_0|^2$ can be identified with the fermion gap Δ. The latter is the order parameter for spontaneous U(1) breaking associated with a superfluid ground state. From the (regularized) grand canonical potential we can derive all thermodynamic observables. Our results for dimensionless (universal) quantities in the unitary limit, such as the critical temperature $T_c/\bar{\mu}$ for the superfluid transition, the gap $\Delta/\bar{\mu}^2$ or the ground-state energy $E/\bar{\mu}$, are independent of $\bar{\mu}$ and g_φ, as expected. To compute the critical temperature T_c, it is convenient to employ the gap equation $(\partial U/\partial\varphi)|_{\varphi_0} = 0$ and exploit the fact that the fermion gap $\Delta \sim \varphi_0^2$ vanishes identically at $T = T_c$.

From Eq. (4), it is apparent that U is 2π-periodic in βh_I when we replace h with ih_I. This is not only true for the mean-field approximation but also for the full theory, as can be seen from Eq. (2) by taking into account that h effectively shifts the Matsubara modes of the fermions $\nu_n = (2n+1)\pi T$. [Note that, loosely speaking, ∂_τ is replaced by $i\nu_n$ when we formulate the action S in momentum space.] It then follows that it is not possible to study arbitrary asymmetries with this technique: h_I is bound to values $\beta h_I < \pi$. However, the proposed approach still allows to study a large part of the phase diagram in the physical (T, h)-plane. We show next that our mean-field results suggest that a (tri)critical point in this phase diagram might indeed be accessible in lattice MC calculations with imaginary h.

In Fig. 1 we show the well-known mean-field phase diagram in the (T, h) plane (see e.g. Refs. [9]). Rather than discussing the appearance of inhomogeneous phases (Sarma and/or FFLO), we only discuss the phase transition lines for homogeneous phases. In Fig. 2, we show the phase diagram in the plane spanned by the temperature and the imaginary-valued polarization. As discussed above, this phase diagram is 2π-periodic in βh_I. We therefore only show the domain $\beta h_I \in [-\pi, \pi]$, which is indicated by the blue dashed lines both figures. Assuming one first computes the phase diagram in Fig. 2, e.g. via lattice MC, we conclude that we would then only have access to the temperature regime $T > h/\pi$ in the physical (T, h) plane of Fig. 1. Nevertheless, this represents a fairly large part of the phase diagram, which is at the heart of theoretical and experimental studies. Most remarkably, our analysis suggests that the (tri)critical point lies within this regime of the phase diagram, i.e. that this point is within the reach of lattice MC calculations with an imaginary asymmetry parameter. The phase transition line can then be obtained from an analytic continuation of the results for $T_c(h_I)$, as we mention below.

The phase structure of the theory in the (T, h_I) plane (Fig. 2) is intriguing. It can be shown analytically that $T_c \to \infty$ for $\beta h_I = (2N+1)\pi$ with $N \in \mathbb{Z}$ and $\bar{\mu} > 0$. This is similar to relativistic fermion models, such as the Gross-Neveu model in $(1+1)d$ [14], and again, we expect this to hold beyond mean field. In fact, instead of the original Matsubara modes $\nu_n = (2n+1)\pi T$, we see from the action (2) that the Matsubara modes of the fermions effectively assume the form $\nu_n = 2n\pi T$ for $\beta h_I = (2N+1)\pi$ usually associated with bosonic degrees of freedom. Thus, the fermions acquire a (thermal) zero mode in this case which tends to condense, independently of the actual value of the temperature. Contrary to relativistic fermion models, however, we find numerically that already $T_c \to \infty$ for $|\beta h_I| > |(\beta h_I)_\infty| = 2.397\ldots$. In other words, there is always a fermion condensate for $|(\beta h_I)_\infty| \leq |\beta h_I| < \pi$ and the U(1) symmetry is not restored at high temperatures in this domain. For $|\beta h_I| < |(\beta h_I)_\infty|$, the phase transition is of second order. The upper bound $|(\beta h_I)_\infty|$ will take a different value beyond the mean-field approximation. In our numerical studies we find that the value $|\beta_{cp} h_{cp}|$ associated with the (tri)critical point is slightly lower than $|(\beta h_I)_\infty|$, in what appears to be merely a coincidence. By studying the weak-coupling regime, one even finds that the difference between $|\beta_{cp} h_{cp}|$ and $|(\beta h_I)_\infty|$ is larger in that regime, at least in mean field [15]. Note that the absence of a (tri)critical point in the (T, h_I) plane as well as the absence of U(1) restoration in the domain $|(\beta h_I)_\infty| \lesssim |\beta h_I| < \pi$ does not imply their absence for the corresponding real-valued asymmetries. In analogy to relativistic fermion models [14], the analytic continuation of the phase boundary gives only the correct behavior up to the (tri)critical point. From the analytic continuation of the (full) order-parameter potential, however, the phase diagram can be mapped out in the physical (T, h)-plane in the whole region where $\beta h < \pi$, including the line of first-order transitions.

As the grand canonical partition function $\mathcal{Z}$, the order-parameter potential U is invariant under $h \to -h$. This allows us to expand $\mathcal{Z}$ (and other physical quantities) in powers of $(\beta h)^2$. In mean-field, we find that the radius of convergence for the grand canonical potential is $r \equiv |\beta h|_{\max} = \pi$ for $\Delta \equiv 0$ and $\bar{\mu} > 0$, but $r > \pi$ in the case of a finite gap Δ. These observations facilitate the analytic continuation from imaginary- to real-valued asymmetry parameter. When performing MC calculations of ultracold Fermi gases, one has now several options to do the analytic continuation. For example, one may fit the data of a given observable $\mathcal{O}$ for a given fixed temperature $T_0 = 1/\beta_0$ to the ansatz $\mathcal{O} = \sum_{n=0}^{N_{\max}} C_{\mathcal{O}}^{(n)} (\beta_0 h_I)^{2n}$, where $C_{\mathcal{O}}^{(n)}$ are constants determined by the fit to the data. $N_{\max}$ represents the truncation order (whose value depends on the amount of data available). Moreover, we have assumed that $\mathcal{O}$ has been made dimensionless with, e.g., a suitably chosen power of $\bar{\mu}$. From a simple analytic continuation of this polynomial, one then obtains the dependence of $\mathcal{O}$ on h.

Within our analytic study, we can check the feasibility of this procedure. For instance, we find that the pressure for $0 \leq \beta_0 h \lesssim 1$ (with $T_0 = 1/\beta_0 \approx \bar{\mu}/2$) can be recovered from a fit to the imaginary-h data with $N_{\max} = 2$. From the pressure one can then in principle compute the ground-state energy as function of h (or, equivalently, the so-called *Bertsch* parameter). However, the zero-temperature values of physical observables for finite $h/\bar{\mu}$ are obviously not directly accessible within such an approach. The *Bertsch* parameter at $h = 0$, on the other hand, is known from lattice MC calculations to approach rapidly its zero-temperature value below the superfluid transition [6]. We see a similar behavior in mean field, even at finite $h/\bar{\mu}$. Therefore it is conceivable that a reliable estimate for the *Bertsch* parameter at $T = 0$ and finite polarization can be extracted from lattice calculations with various different temperatures and a subsequent analytic continuation of the data.

Instead of a simple Taylor expansion, one may employ more elaborate fit functions such as Padé approximants, also used in lattice QCD studies [11]. In Fig. 1, for example, we have reconstructed the phase boundary at real-valued asymmetry by fitting the phase transition line in the $(\beta h_{\rm I}, \beta\bar{\mu})$-plane with the function

$$C \frac{1 + \sum_{i=1}^{N_{\max}} a_i [1 - \cos(\beta h_{\rm I})]^i}{1 + \sum_{j=1}^{N_{\max}} b_j [1 - \cos(\beta h_{\rm I})]^j} \,, \qquad (5)$$

where $N_{\max}$ again defines the truncation order. The a_i's, b_i's and the constant C are determined by the fit. This ansatz already respects the 2π-periodicity of the theory in $\beta h_{\rm I}$ and can be generalized to observables other than $T_{\rm c}$. In Fig. 1 we show our results for the critical temperature $T_{\rm c}$ from such a fit for $N_{\max} = 1, 2, \ldots, 5$, see Ref. [15] for details. Finally, we note that the fits may be even further optimized by choosing even more elaborate sets of basis functions [16].

We have completely left out the discussion of inhomogeneous phases and whether these phases also appear in the $(T, h_{\rm I})$ plane. While such a discussion is left to future work, we do not expect an inhomogeneous condensate $\varphi_0(\vec{x}) \sim {\rm e}^{{\rm i}\vec{q}_0\cdot\vec{x}}$ to show up in its well-known form, where the (center-of-mass) momentum $\vec{q}_0$ is determined by the difference in the chemical potentials of the spin-up and spin-down fermions. From a very simple point of view, one may naively expect that the solutions $\varphi_0(\vec{x})$ of the quantum equation of motion turns into $\varphi_0(\vec{x}) \sim {\rm e}^{-\vec{q}_0\cdot\vec{x}}$ for complex-valued chemical potentials and might then no longer define the ground state.

We have discussed the possibility of studying polarized Fermi gases with the aid of complex-valued chemical potentials. While the latter are not required in analytic studies, they are in MC calculations which would otherwise be spoiled by the sign problem. We have argued that the (tri)critical point is in principle within reach in this framework and the zero-temperature limit of observables might be indirectly accessible as well. This work therefore suggests that, together with the experimental data at hand, future *ab initio* MC calculations with complex-valued chemical potentials have the capacity to push our understanding of collective many-body phenomena to a new level. Our present study marks the starting point and can already be used to guide these calculations.

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